Release Files for ENDF/B-VII.0.fix1

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MCNP ENDF70 Library

- All ENDF/B-VII.0 neutron materials, except 3
  - Be-7
  - Cf-253
  - Es-253
- Processed at 5 temperatures
  - 293.6 K
  - 600 K
  - 900 K
  - 1200 K
  - 2500 K
- Released as part of MCNP5 1.50 package

Modifications Made to Eight ENDF/B-VII.0 Evaluations

1. H-1
2. Sc-45
3. Y-89
4. Zr-96
5. Mo-97
6. Eu-153
7. Am-242g
8. Am-242m

Modifications

- H-1
  - The only change we made to ENDF/B-VII.0 before processing for MCNP was to modify the energy of the gamma from radiative capture from 2.2246 MeV to 2.2233 MeV. This change had been made in ENDF6.8, but the value reverted to 2.2246 in ENDF7.0. The explanation for the difference is that the 2.2246 MeV value is the total energy, whereas 2.2233 MeV is the actual energy of the gamma – the difference going in to recoil energy.

Modifications

- Sc-45
  - The ENDF/B-VII.0 evaluation had angular distributions for MTs 16, 22, 28, and 91 originally specified in the center-of-mass system. NJOY / CONSIS caught this and complained about it. We changed the reference frame to Laboratory system for those four reactions.
  - In addition, MF=13 MT=3 has an illegal non-zero cross section at threshold (if it is not illegal -- it should be!!). The first value in the cross section tabulation is at 1 MeV with a cross section of .91172 barns. Bad - very bad! We changed this so that point 1 had an energy of 0.999999 MeV and a cross section of zero, and point 2 had an energy of 1.000001 MeV and a cross section of .91172 barns.

Modifications

- Y-89
  - MT=91 had negative cross sections from ~ 1.7 MeV through 4.1 MeV.
  - Our fix to the evaluation was to zero out MT=91 all the way from its original threshold of 0.99 MeV to 4.06844 MeV. Above this value, we used the original (positive) values from the evaluation for MT=91.
  - This should definitely be looked at by the evaluators and not accepted as the right fix. The negative numbers that were originally in MT=91did force a balance so that MT=4 equaled the sum of MTs 51-91. Was MT=4 also wrong? Is the whole inelastic scattering suite of cross sections wrong?

Modifications

- Zr-96 and Mo-97
  - For both Zr96 and Mo97, NJOY/CONSIS gives:

    "consis: bad law44 kalbach r for (n,xp) at 1.800000E+01 ......
    1.900000E+01
    2.000000E+01"

  - The issue is that a value of 0.999999E+01 or so appears (instead of 9.99999E-01 or 0.999999E+00) for energies of 18, 19, and 20 MeV in mf=6 mt=204 for Zr96 and mt=203 for Mo97.
  - We changed the r values to be 9.99999E-01 instead of 0.999999E+01

Modifications

- Eu-153
  - This evaluation in ENDF/B-VII.0 had numerous negative pdf's (for probability of scattering to specific secondary neutron energies) in MF6 MT91 at neutron energies from 16 - 20 MeV. We actually did not create a modified ENDF format file; rather we simply replaced the negative pdf's with zeros in the MCNP file and renormed the distributions to unity.
  - It should be noted that these were not trivial negative values as the distributions had to be renormalized by ~ 2 - 2.5%.

Modifications

- Am-242g
  - The VII.0 evaluation for Am-242 did not provide any angular distribution information for MT=18 (there was no MF=4 MT=18 and no MF=6 MT=18). This actually causes NJOY to produce an MCNP ACE file that is wrong.
  - We rectified the problem by providing an updated version of the Am-242 evaluation that had a simple isotropic MF=4 MT=18 subsection added.

Modifications

- Am-242m
  - Am-242m had unexpected behavior in inelastic scattering for MTs 4, 51, 52, 53, and 54. Cross sections were non-zero from 20 keV (or threshold) up to 50 keV, then were zero from 50 keV to 65 keV, and then non-zero again above 65 keV.
  - Patrick Talou provided us with updated values for these inelastic channels between 50 and 65 keV. We created the ENDF70 library based on Patrick's updated data.

Status

- Updated ENDF6 format files have been sent to NNDC for seven of the eight evaluations
  - H-1, Sc-45, Y-89, Zr-96, Mo-97, Am-242, and Am-242m
- I need to create and send the updated file for Eu-153

U-233 Delayed Neutron Error

- ENDF/B-VII.0 delayed fission nubar:

Nubar table: eV nubar eV nubar eV nubar
---------- ---------- ---------- ---------- ---------- ----------
1.000000-5 7.400000-3 4.500000+6 7.400000-3 6.000000+6 4.700000-3
1.400000+7 4.700000-2 1.500000+7 4.200000-2 3.000000+7 4.200000-2

- This is identical to ENDF/B-VI.
- Bob MacFarlane believes that the values at 14, 15, and 20 MeV should be decreased by an order of magnitude.
- We did not make this change in ENDF70.

S(α,β) Processing

- Not trivial to create MCNP S(α,β) tables with NJOY
  - THERMR "ICOH" entry
    - Needs to be non-zero for all moderators that have elastic scattering; not just for the specific moderators listed in the NJOY manual.
    - Solid methane, Fe56, Al27, O and U in UO_2
  - THERMR "NATOM" entry and ACER "NMIX" entry
    - Make sure that the elastic cross section at "high" energies in the thermal table converges to proper value
  - What isotopes are evaluations appropriate for?
    - Benzene is only ENDF/B-VII.0 evaluation intended for more than one element (H and C).
    - What about Fe56 and Al27? U in UO_2 just for U-238?
  - We will provide our NJOY processing values used to create ENDF70SAB to the NNDC for posting